Spin-dependent thermoelectric transport coefficients in near-perfect quantum wires

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Thermoelectric transport coefficients are determined for semiconductor quantum wires with weak thickness fluctuations. Such systems exhibit anomalies in conductance near 1/4 and 3/4 of $2e^2/h$ on the rising edge to the first conductance plateau, explained by singlet and triplet resonances of conducting electrons with a single weakly bound electron in the wire (T. Rejec, A. Ramšak, and J.H. Jefferson, Phys. Rev. B **62**, 12985 (2000)). We extend this work to study the Seebeck thermopower coefficient and linear thermal conductance within the framework of the Landauer-Büttiker formalism, which also exhibit anomalous structures. These features are generic and robust, surviving to temperatures of a few degrees. It is shown quantitatively how at elevated temperatures thermal conductance progressively deviates from the Wiedemann-Franz law.

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I. INTRODUCTION

One of the main properties of small confined electron systems, intensively studied experimentally and theoretically in the last decade, is the electrical conductance. However, other transport coefficients also serve as a sensitive probe of new phenomena in such systems, such as the thermopower of chaotic quantum dots [1] or of atomic size metallic contacts [2] and most recently, anomalies in one-dimensional wires [3]. Theoretical investigations predict in these systems a range of new properties of transport coefficients, such as anomalously enhanced thermopower in quantum dots due to the Kondo effect [4] and, at low temperatures, changes in sign together with linear thermal conductance violating Wiedemann-Franz law [5]. Anomalies in thermoelectric coefficients are also found in standard strongly correlated systems: the Anderson model [6], the Hubbard model [7] and the t-J model [8].

In this paper, we extend our recent theoretical study of conductance anomalies to include thermoelectric effects due to a temperature gradient. Anomalies are related to weakly bound electron states within the quantum wire. In particular, we consider a small fluctuation in thickness of the wire in some region giving rise to a weak bulge. If this bulge is very weak then only a single electron will be bound. We may thus regard this system as an 'open' quantum dot in which the bound electron inhibits the transport of conduction electrons. Near the conduction threshold, there is a 'Coulomb blockade' and we have shown that this gives rise to spin-dependent resonances, also in an axial magnetic field, for wires of both rectangular [9] and cylindrical [10] cross-section.

Experimentally, the staircase structure of the conductance of quantum wires was reported more than a decade ago [11], and more recent systematic investigations showed unexpected structure in the rising edge to the first conductance plateau [12–15].

Here we model a quantum wire as in Ref. [10] and, explicitly, we assume a wire of circular symmetry about the z-axis with constant potential, $V(r,z)=0$ within a boundary $r_0(z)$ from the symmetry axis and confining potential $V_0>0$ elsewhere. This geometry is close to that of narrow 'v'-groove quantum wires, which also exhibit anomalies near the conductance threshold [15]. To be definite, we choose parameters appropriate to GaAs for the wire and Al_xGa_{1-x} As for the barrier with x such that $V_0=0.4$eV, which is close to the crossover to indirect gap. The wire width is taken as $r_0(z)=\frac{1}{2}a_0(1+\xi\cos^2\pi z/a_1)$ for $|z|\le\frac{1}{2}a_1$ and $r_0(z)\equiv\frac{1}{2}a_0$ otherwise, i.e., a wire of width a_0 with a single bulge of length a_1 and width $(1+\xi)a_0$, as shown in insets of Fig. 1(c) and Fig. 2(c).

II. CONDUCTANCE

We consider the interacting electron problem with the above wire thickness variation in a range which ensures that only one electron occupies a bound state and that restriction to a single channel near the conduction edge is an excellent approximation. This is always the case for a very weak smooth variation, i.e. a near perfect wire. From numerically exact solutions of the two-electron scattering problem, the conductance is calculated from our generalisation of the usual Landauer-Büttiker (LB) formula [16], to include spin-dependent scattering [17] of conduction electrons from the single electron bound in the potential well. This gives $G(\mu)=G_0\ \mathcal{T}(\mu)$, where

$G_0 = 2e^2/h$, μ is the Fermi energy and the transmitivity is a weighted average over singlet and triplet channels [9,10,18],

$$\mathcal{T}(\mu) = \frac{1}{4}\mathcal{T}_{\rm s}(\mu) + \frac{3}{4}\mathcal{T}_{\rm t}(\mu). \tag{1}$$

At elevated temperatures we use the LB finite temperature extension

$$G(\mu) = G_0 \int \left[-\frac{\partial f(\epsilon,\mu,T)}{\partial \epsilon} \right] \mathcal{T}(\epsilon) d\epsilon, \tag{2}$$

where $f(\epsilon,\mu,T) = (1+\exp[(\epsilon-\mu)/k_{\rm B}T])^{-1}$ is the usual Fermi function which describes the thermal distribution of electrons in the leads. $G(\mu)$ is shown in Fig. 1(a) and Fig. 2(a) for a wire with relatively small and a larger bulge, respectively. Here the energy is measured from the threshold of the conductance. As discussed in Ref. [10], the weak bulge in the wire is equivalent to a shallow potential well in a perfectly straight wire and if the length of the bulge region is small, this effective potential well can only accommodate one bound state with the consequence that only a singlet resonance in G exists, as observed, for example, in Ref. [15]. Conversely, if the bulge region is longer, both, singlet and triplet resonances contribute. For even longer bulge regions with a very shallow effective potential well (near perfect wire), the singlet resonance is pushed to lower energy and therefore becomes extremely narrow. In this regime, only the broader triplet can be resolved at finite temperature [9,10], as observed experimentally in clean gated structures [12–14].

III. THERMOELECTRIC EFFECTS

The LB approach can be extended to include electrical and heat currents through a region between two leads with different temperatures and chemical potentials [19,20]. With $T+\Delta T$, $\mu + eU$ for the left lead and T, μ for the right lead, we get

$$j = \frac{2e}{h}\int \Delta f(\epsilon)\mathcal{T}(\epsilon){\rm d}\epsilon, \tag{3}$$

$$j_{\rm Q} = \frac{2}{h}\int (\epsilon-\mu)\Delta f(\epsilon)\mathcal{T}(\epsilon){\rm d}\epsilon, \tag{4}$$

and

$$\Delta f(\epsilon) = f(\epsilon, \mu+eU, T+\Delta T) - f(\epsilon,\mu,T). \tag{5}$$

In the linear response regime of vanishing ΔT and U the currents simplify to

$$j = \frac{2e^2}{h}K_0(\mu)U + \frac{2e}{h}K_1(\mu)\frac{\Delta T}{T}, \tag{6}$$

$$j_{\rm Q} = \frac{2e}{h}K_1(\mu)U + \frac{2}{h}K_2(\mu)\frac{\Delta T}{T}, \tag{7}$$

where

$$K_n(\mu) = -\int (\epsilon-\mu)^n \frac{\partial f(\epsilon,\mu,T)}{\partial\epsilon}\mathcal{T}(\epsilon){\rm d}\epsilon. \tag{8}$$

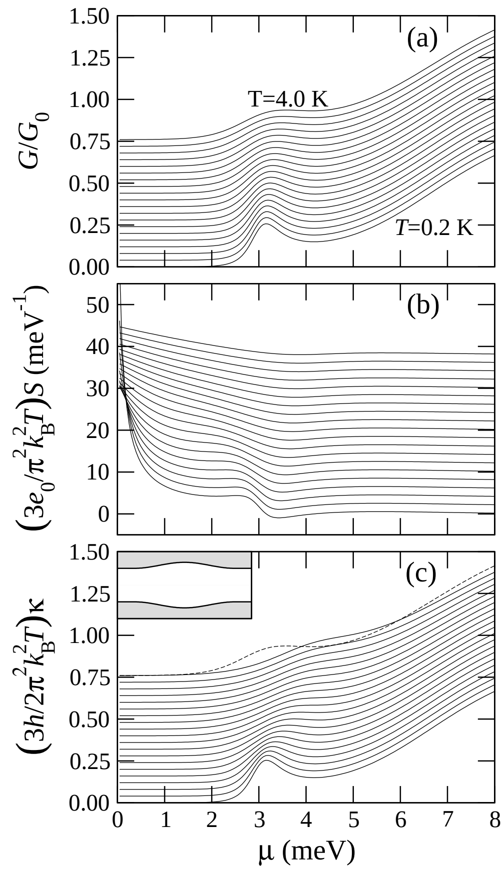

FIG. 1. (a) Electrical conductance $G(\mu)$, (b) thermopower $S(\mu)$, and (c) thermal conductance $\kappa(\mu)$ for wire parameters a_0 = 10 nm, a_1 = 30 nm, ξ = 0.18 and screening length ρ = 100 nm. Other parameters and the numerical method is as in Ref. 10. The dashed line in (c) represents Wiedemann-Franz law result for T = 4K. The traces for different T are offset vertically for clarity.

A. Thermopower

The Seebeck thermopower coefficient S measures the voltage difference needed to neutralize the current due to the temperature difference between the leads. In the linear response regime the thermopower is given by,

$$S(\mu) = \frac{U}{\Delta T} = -\frac{1}{eT}\frac{K_1(\mu)}{K_0(\mu)}, \tag{9}$$

as is for various systems discussed in Refs. [20,3]. Eq. 9 is formally the same as the Mott-Jones formula for simple metals [21] and generalized for a system with stronger electron-phonon interactions in Refs. [22].

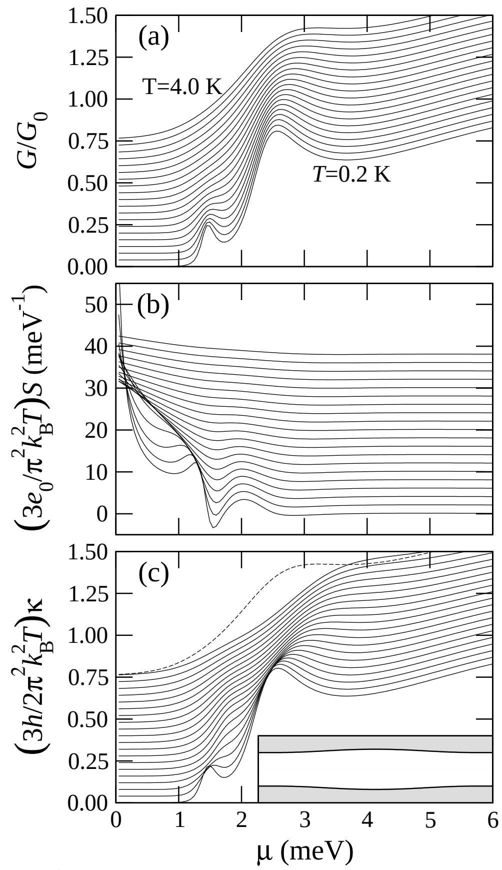

FIG. 2. As Fig.1, but for longer bulge with parameters $a_0 = 10$ nm, $a_1 = 60$ nm and $\xi = 0.1$.

In Fig. 1(b) the thermopower of a narrow wire with a small bulge is presented for the same range of temperatures as $G(\mu)$. Such a result is expected, e.g., for the system studied in Ref. [15]. The structure reflects the singlet resonance observed in the conductance and is smeared out at temperatures comparable with the width of the resonance. In a wire with small thickness variation, but with a longer bulge, triplet resonance scattering also exists, as shown in Fig. 2. In the thermopower curve of Fig. 2(b), the dominant structure at lower temperatures comes from the singlet resonance, though the triplet resonance is still clearly discernible. At higher temperatures the triplet structure is washed out first, in contrast to the conductance result, Fig. 2(a). At low temperatures only the transmitivity at energies close to the chemical potential contributes to the above integrals and the general result Eq. 9 can be related to the temperature dependent $G(\mu)$ by the following expansion

$$S(\mu) = -\frac{\pi^2 k_{\rm B}{}^2 T}{3e}\left(\frac{\partial \ln G(\mu)}{\partial \mu} + \frac{\pi^2 k_{\rm B}^2 T^2}{15\, G(\mu)}\frac{\partial^3 G(\mu)}{\partial \mu^3}\right) + \cdots \tag{10}$$

Our results were calculated using the exact relation Eq. 9. However, the leading term in Eq. 10, is a reasonable approximation for energies above the singlet resonance and up to temperatures where the structure is thermally smeared out. This is shown in Fig. 3(a) where we present a comparison of $S(\mu)$ for the exact result with the approximations to first and second order. We see that at energies below the resonance, both the linear and cubic approximations deviate significantly from the exact result, Eq. 9. In this regime the conductance is itself very small and hence $G(\mu)^{-1}\partial^n G(\mu)/\partial \mu^n$ is prone to error making calculations and experimental data analysis based on this expansion unreliable.

The thermopower of one-dimensional wires has been measured [23,24] and more recently, further anomalies related to '0.7 anomaly' in conductance were reported [3]. The authors of Ref. [3] observe a dip in $S(\mu)$ at energies corresponding to the anomaly in $G(\mu)$. However, the logarithmic derivative with respect to the gate voltage of the measured G exhibits a much deeper minimum than the dip in the measured $S(\mu)$, which remains well above zero even at the lowest temperatures . This clearly shows that a simple non-interacting formula is not valid in this low temperature regime. Apart from the small corrections to the logarithmic approximation to S, our model and its solution within the LB framework are

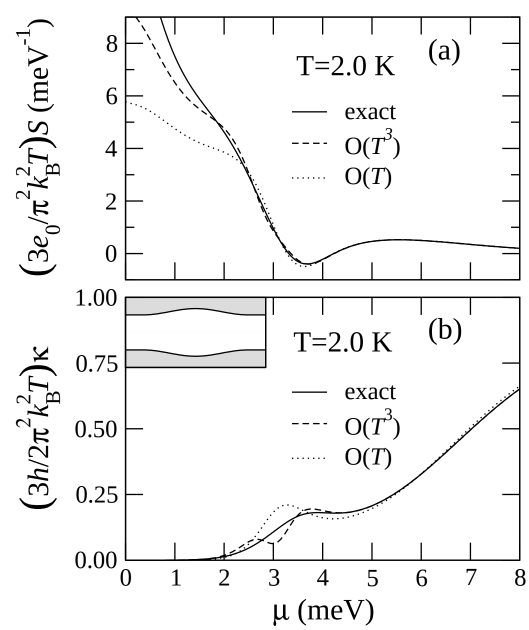

FIG. 3. (a) Thermopower as obtained with Eq. 9 for $T = 2$K and parameters used for Fig. 1 (full line). Dashed and dotted lines correspond respectively to the result of Eq. 10 and the linear T approximation (first term in Eq. 10). (b) Thermal conductance – parameters as in (a).

in agreement with the findings of Ref. [3]. That is, the calculated thermopower is in good agreement with experiment except at low temperatures where we also predict a deep minimum. This discrepancy at low-temperatures may well be a many-body Kondo-like effect contained within our model but not within the two-electron ap-

proximation we have used here and in our earlier papers. We expect the two-electron approximation to break down at low temperatures for which the underlying extended Hubbard model, which is the starting point of our approach, can be mapped onto a generalised Anderson model with coupling terms that are strongly energy dependent [25]. The standard results for the single impurity problem [6] cannot be applied directly to this effective model, which is the subject of current research [26]. At very low temperatures, a Kondo-like resonance is expected [5], for which many-body effects would dominate with a breakdown of formula Eq. 9.

B. Thermal conductance

The linear thermal conductance is the heat current divided by the temperature difference between the leads when the chemical potentials are adjusted to give no electrical current. From Eqs. 6-8 we see that this is related to $\mathcal{T}(\epsilon)$ by,

$$\kappa(\mu) = \frac{2}{hT}\left(K_2(\mu) - \frac{K_1^2(\mu)}{K_0(\mu)}\right). \tag{11}$$

For low temperatures this simplifies to Wiedemann-Franz law, first term in

$$\kappa(\mu) = \frac{\pi^2 k_{\mathrm{B}}^2 T}{3e^2} G(\mu)\Bigg(1 + \tag{12}$$
$$+ \frac{\pi^2 k_{\mathrm{B}}^2 T^2}{15}\left[\frac{8}{G(\mu)}\frac{\partial^2 G(\mu)}{\partial \mu^2} - 5\big(\frac{\partial \ln G(\mu)}{\partial \mu}\big)^2\right]\Bigg) + ...$$

In Fig. 1(c) and Fig. 2(c) $\kappa(\mu)$ is shown for T from 0.2K to 4K, calculated from Eq. 11. Comparison of Figs. 1(a),2(a) with Figs. 1(c),2(c) shows good agreement with the Wiedemann-Franz law at lower temperatures but there is increasing deviation at higher temperatures in the resonance region. For comparison, the dashed lines in Fig. 1(c), Fig. 2(c) show the corresponding linear approximation result, Eq. 12. This is also seen in the plot of κ for $T = 2$K shown in Fig. 3(b). One of the most striking features of these plots is that $\kappa(\mu)$, calculated from Eq. 11, exhibits an anomaly at higher energies than the corresponding anomaly in conductance, a prediction which is open to experimental verification.

IV. SUMMARY

In summary we have, within the framework of the LB approach, calculated thermal transport coefficients for near-perfect quantum semiconductor quantum wires, extending our earlier work on spin-dependent conduction anomalies. These anomalies are a universal effect in one-dimensional systems with very weak longitudinal confinement. The emergence of a specific structure $G(\mu) \sim \frac{1}{4}G_0$ and $G \sim \frac{3}{4}G_0$ is a spin effect, being a direct consequence of the singlet and triplet nature of the resonances. The probability ratio 1:3 for singlet and triplet scattering follows directly from this and as such is a universal effect, not only for conductance but all thermoelectric transport coefficients. A comprehensive numerical investigation of open quantum dots using a wide range of parameters shows that singlet resonances are always at lower energies than the triplets, in accordance with the Lieb-Mattis theorem for bound states [27].

Thermopower plots show anomalies, related ultimately to the Coulomb interaction between a localised electron and the remaining conduction electrons. We have shown that the lower-energy singlet anomalies in thermopower are more pronounced. These should be clearly observable in wires which show the corresponding conductance anomalies, such as the narrow 'hard confined' wires reported in Ref. [15], or in gated quantum wires under high source-drain bias where the singlet anomaly is clearly observed [28].

Finally we conclude by emphasising that although our model of a quantum wire with a weak bulge may appear rather specialised, it is actually quite general since the weak bulge is mathematically equivalent to a weak potential well in an otherwise perfect wire. As with our previous work, we have not investigated in detail the actual causes of such weak effective (or real) potential wells but point out that they may well be due to quite different sources in different experiments, e.g. thickness fluctuations, remote impurities or gates, electronic polarisation, or some other more subtle electron interaction effect. The main point is that because the effective potential well is shallow, *it will bind one and only one electron.* The universal anomalies in conductance and thermopower are a direct consequence of this and occur for a wide range of circumstances in almost perfect quantum wires.

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